Jan 6, 2014 10:40 AM EB1 - Room 1011	**Professor Phillip R. Westmoreland** Department of Chemical and Biomolecular Engineering

Opportunities and Challenges for a New Golden Age of Chemical Engineering

In my year as AIChE president, I saw amazing things happening in our profession around the world. I propose that we are in the early days of a new "Golden Age" of chemical engineering and cite five reasons.

First is new availability of energy supplies worldwide through hydrofracturing and renewable energy. Meanwhile, molecular biology has become a promising tool for production of chemicals and medicines. Computing advances aid our understanding and applications of molecular science, along with product design and process operation. Fourth, manufacturing is more process-oriented than ever, benefiting from chemical-engineering expertise. Finally, the molecular, systems, and process-based approaches of chemical engineering are well suited to addressing society's needs and aspirations.

These changes provide new opportunities and new challenges, as I will show by recent examples. The late John Chen recently examined how academic preparation and industry needs can diverge unless we have common acceptance of what ChE fundamentals are. A key to our potential impact is embracing the breadth and core of our professional identity as chemical engineers.

Jan 13, 2014 10:40 AM EB1 - Room 1011	**Dr. Michael Tam** University of Waterloo, Canada

Cellulose Nanocrystals and Amphiphilic Polymers: Functionalization, Characterisation and Applications in Chemical & Biomedical Systems

Nanotechnology is anticipated to be the next technological wave that will drive many of the innovations in science and engineering. In this discipline, there is a renewed impetus to develop nanomaterials from renewable sources due to the negative impact of using raw materials from traditional carbon sources, such as crude oil.

New opportunities in the use of sustainable and renewable materials for chemical and biomedical sciences exist, and CNC offers a new route to product development and formulations in this industrial sector.

The talk will focus on the important role CNC functionalization plays in imparting attractive properties that are critical for their applications. For example, functionalization of CNC with fullerene and amphiphilic polymers was performed. Special focus will be devoted to the physical interactions between CNC and various amphiphilic compounds, and how these interactions impact their stability and microstructure. In order to fully elucidate the microstructural evolution of CNC/surfactant interactions, rapid and robust characterisation techniques for quantifying the evolving molecular structure are used to elucidate their morphologies and microstructure.

I will end my presentation with some comments on the future directions and new opportunities of CNC in other related market sectors.

Feb 3, 2014 **10:40 AM** **EB1 - Room 1011**	**Pablo Debenedetti** Department of Chemical and Biological Engineering - Princeton University
McCabe Lecture - Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality	
Chiral asymmetry choices exhibited by molecules in living organisms (e.g. amino acids and sugars) constitute a scientifically challenging set of observations. We have formulated thermodynamic and kinetic models of chiral amplification that provide insight into possible scenarios for the emergence of chiral imbalance in the prebiotic world. The thermodynamic model involves enantiomeric forms of a chiral molecule and a non-chiral liquid solvent. Thermodynamic equilibrium of the modeled system results in liquid-phase chiral amplification, in agreement with experimental observations. Numerical solution of the kinetic model identifies two regimes. In one, the system evolves towards a mixture containing equal amounts of the chiral enantiomers. In the other, the system evolves towards large excess of one of the chiral enantiomers. Results will also be presented on a kinetic Monte Carlo model that reproduces experimental observations on attrition-enhanced chiral symmetry breaking, of relevance to the separation of chiral compounds in the pharmaceutical industry.	

Feb 10, 2014 **10:40 AM** **EB1 - Room 1011**	**Dr. Keisha Walters** Mississippi State University
Material design . . . from molecule to function: Stimuli-responsive polymers and polymer-metal nanocomposites	
Stimuli-responsive polymers (SRPs) substantially alter their physical properties (e.g., shape and viscosity) in response to environmental triggers (e.g., temperature, pH, solvent quality). These next-generation materials show significant potential to transform applications in medicine, sensors, self-healing materials, and environmental remediation. In this talk, I will discuss methods for building SRPs in bulk and tethered to a substrate. Well-controlled syntheses can allow for targeted selection of chemical composition, molecular weight, and ultimately the stimulus condition and associated relative change in properties. SRP-metal nanocomposites offer inherent advantages in terms of being able to fine-tune nanostructure surface chemistry, integrate multiple (potentially disparate) materials, and dynamically assemble 2- and 3-dimensional structures. Characterization of several SRP-metal nanocomposite systems will be presented in the context of their intended applications.	

Feb 17, 2014 10:40 AM EB1 - Room 1011	**Dr. Ryan Gill** University of Colorado

The Genome Design-Build-Test Shop

The era of genome engineering has arrived. Synthetic DNA technologies can now generate sufficient DNA to construct tens of thousands of genes in parallel; enough to synthesize several complete microbial genomes at the same time. Genome sequencing has advanced to the point where such genomes can be completely sequenced in < 1 day for about <$1000 using a benchtop sequencer.

These technologies were used in the creation of the first synthetic genome. Such genome-construction technology was first applied to the copying of existing genomes, thus avoiding any significant design phase. Future applications will seek to develop artificial genomes that will be designed to encode industrially relevant functions; such as production of biofuels, sustainable chemicals, pharmaceuticals, industrial enzymes, etc. Such applications will require that we are able to not only identify genes encoding functions that enable such applications but also combinations of such genes, and combinations of such combinations, that together result in optimal organism performance.

We are developing a range of new technologies for designing genomes based upon the i) construction and use of ideal chassis strains, ii) efficient identification of gene-to-phenotype design rules, iii) automated rational combinatorial mutation library generation, and iv) parallel interrogation of such libraries to identify combinatorial design rules.

This presentation will describe the first generation of such technologies, the current state of next-generation approaches, and the most recent application of such tools to design and construct microbial genomes relevant to sustainable fuels and chemicals production.

Feb 17, 2014 2:30 PM Room 2207 EB3	**Dr. Elizabeth Nance** Center for Nanomedicine - Johns Hopkins Medical Institutions

Nanotherapeutics for Brain Diseases

Nanotechnology-based approaches provide potential platforms for site-specific controlled, sustained release of therapuetics for central nervous system (CNS) diseases. Nanoparticles can safely enhance therapeutic delivery to disease sites and provide sustained, well-dispersed drug delivery into the regions of the brain that contain diffuse diseased cells, and may find use in the treatment of many CNS diseases, including those involving neuroinflammation. Neuroinflammation, mediated by activated microglia and astrocytes, plays a key role in the pathogenesis of many neurological disorders, including Alzheimer's, autism, cerebral palsy (CP), and traumatic brain injury (TBI). Recent literature has implicated activated microglia/astrocytes in neurodegenerative diseases, and suggests that attenuating neuroinflammation in the early stages can not only delay the onset, but may also provide a longer therapeutic window for treatment. Targeting activated microglia/astrocytes may offer such an opportunity. However, this is a challenge on multiple levels because (1) transport of drugs and drug delivery vehicles across the blood-brain-barrier (BBB) is difficult to achieve, (2) injury is often diffuse, making it difficult for therapeutics to reach target cells even if administered locally, and (3) the effect of changes in the extracellular matrix, brain edema, glial cell function and BBB disruption on the movement, interactions, and cellular uptake of nanoparticles, especially in the developing brain, is not well understood.

My research goals focus on understanding nanoparticle platform interaction within neuroinflammation-associated disease physiology, to better design and implement therapeutic nanoparticle platforms in clinically relevant models of CNS disorders. This seminar will focus on the following: (i) understanding limitations of polymeric nanoparticle movement within normal and diseased brain and implications following local delivery, (ii) in vivo brain distribution and cell-specific uptake of dendrimer nanoparticles following systemic delivery, and (iii) therapeutic application of dendrimer nanoparticles to achieve efficacy in pediatric brain disease. The long term objectives of this work are to (i) determine the impact of disease etiology and progression on the design of a therapeutic nanoparticle platform, (ii) develop nanotherapeutic applications in clinically relevant animal models of brain injury and (iii) provide insights into the role of modulating cell activation and chronic neuroinflammation in developmental disorders. This is the first body of work to bring nanotherapeutic approaches to perinatal/neonatal brain injury, with an analysis and understanding of the developmental biology and pathology associated with disease, with implications that can be translated to adult brain disease.

Feb 24, 2014 10:40 AM EB1 - Room 1011	**Dr. M. Scott Shell** University of California, Santa Barbara

Simulation Insights into Designer Self-Assembled Materials

We discuss the development and application of novel molecular simulation methods to understand bio-inspired self-assembly principles in nanostructured materials. In the first part of the talk, we consider newly engineered peptides that hold promise as controllable, environmentally benign alternatives for nanoscale materials and scaffolds. Despite experimental advances in this area, it remains an immense challenge to predict even basic self-assembly properties from a theoretical perspective.

We show how novel multiscale simulation techniques can elucidate the delicate balance of assembly driving forces and modulate novel emergent phase behavior in these systems.

In the second part of the talk, we examine self-assembly as route to chiral materials made from achiral molecules. We show that a surprisingly simple mechanism, based only on excluded volume interactions, can drive achiral particles into chiral assemblies. The mechanism quantitatively explains recent experimental results reporting emergent chirality in the two-dimensional hard triangle system, and it predicts other shapes that might exhibit similar behavior.

Such results suggest a potentially powerful new knob for designing materials with unique chiral responsive behavior, and may also suggest a way that chiral structures might emerge in nature.

Mar 3, 2014 10:40 AM EB1 - Room 1011	**Dr. Ian Schneider** Iowa State University

Roles for Mechanical and Biophysical Cues in the Tumor Microenvironment

The tumor microenvironment is complex, consisting of various cell types that shape its mechanical and biophysical properties through the assembly of fiber networks. Entangled, crosslinked fiber networks require tumor cells to activate degradative enzymes called proteinases. Aligned fibers direct tumor cell migration into the surrounding tissue. I will present our recent work focused on distinct but related processes: fiber network degradation and directed cell migration.

First, I will present work using fluorescent probes to measure proteinase activity around tumor cells. Our data suggest that tumor cells detect collagen fiber crosslinks by sensing mechanical properties using intracellular contractile force. This allows them to tune the activity of proteinases based on the mechanical properties and crosslink density of the surrounding fiber network.

Second, I will present work using an exquisitely tunable system by which to organize collagen fibers on mica substrates. Our data suggests that intracellular contractile force, which may differ among different tumor cell lines, dramatically modulates the cell's ability to move along aligned collagen fibers.

Finally, I will briefly describe our future efforts in engineering 3D co-culture environments to examine how tumor and normal cells communicate through mechanical and biophysical signals. It is tempting to envision a future where therapies to fix or diagnostics to sense mechanical or biophysical properties complement the more traditional use of biochemical targets and markers in oncology.

Mar 17, 2014 10:40 AM EB1 - Room 1011	**Dr. Jon-Paul Maria** NCSU

Surfactant-assisted physical vapor deposition: new approaches for improving complex oxide thin film growth

Epitaxial integration of complex oxides with wide band gap polar semiconductors such as GaN (0002) presents the possibility for high-power, high-frequency, and high temperature GaN electronics by virtue of 2-D charge carriers at polar interfaces and possible access to non-linear dielectric properties.

This work describes synthesis and characterization of such thin film heterostructures by MBE, with specific attention given to controlling film growth. We will show that while perfectly lattice matched (111) oriented MgO-CaO solid solution films can be grown on GaN, the terminal surface is always faceted and rough. This unwanted morphology, is determined by the tendency for the high-energy (111) polar orientation to form (100)-oriented low-energy facets, and the interfacial symmetry between cubic MgO and hexagonal GaN.

To overcome this limitation and to realize atomically smooth oxide films on GaN we introduce an *in situ* surfactant growth method. In this method, one introduces a small flux water vapor during MBE growth to hydroxylate CaO and MgO (111) surfaces *in situ*. This changes the equilibrium habit from cubic to octahedral, eliminating the (100) faceting tendency. RHEED oscillations and AFM images of these films show 2D growth, suggesting that altering the surface chemistry during growth plays a critical role in determining the surface orientation.

We demonstrate through electrical property measurements the impact of smooth (111) rocksalt surfaces as leakage current densities for thin CaO films are reduced by two orders of magnitude when films of equivalent thickness are grown using a 2-D vs. a 3-D mode. We also present a set of temperature *ab-initio* thermodynamic calculations of rocksalt oxide surface energies with and without H-containing terminations that validate the surface-chemical mechanism of facet stabilization.

Mar 17, 2014 2:30 PM BTEC - Room 135	**Dr. Moti Herskowitz** Blechner Center for Industrial Catalysis and Process Development, Ben-Gurion University of the Negev

Catalytic Technologies are Expected to Dominate Production of Synthetic Liquid Fuels from Renewable and Alternative Sources by Catalytic Processes

CBE/BTEC Joint Seminar

Synthetic liquid fuels produced from renewable and alternative feedstocks are essential components of the future energy outlook, mainly for transportation. The potential feedstocks for large-scale production of synthetic fuels are divided into three groups: fossil (natural gas and coal), biomass and carbon dioxide combined with hydrogen from water. Processing crude oil in refineries is dominated by catalytic technologies. Conversion of natural gas and coal is mostly practiced through a combination of two processes: catalytic gasification and Fischer-Tropsch synthesis (FTS). Biomass is converted to liquid fuels by thermal, catalytic and biological processes available in the market or being developed. The first generation technologies for production of fuels from edible feedstocks (corn, vegetable oils) are being replaced by the second generation technologies based on non-edible feedstocks.

The Blechner Center (http://www.bgu.ac.il/indcat/) has developed, over the past two decades, infrastructure and expertise required to deal with a wide variety of challenging projects in the area of fuels in general and renewable fuels in particular. Specifically, it has developed a novel process for converting vegetable and algae oils to advanced green diesel and jet fuels. The Blechner Center is developing an integrated catalytic system for conversion of mixtures of CO2/CO/H2 to hydrocarbons that are readily converted to jet and gasoline fuels. The renewable hydrogen could be produced from water by various splitting technologies. Novel catalytic Fe-based materials combined with a novel design of the process yielded excellent, unprecedented performance. CO2 conversions as high as 90% were obtained, reaching high selectivity to liquid (C5+ hydrocarbons), well-beyond reported results in the scientific and patent literature.

This presentation will focus on existing and foreseeing catalytic processes for converting alternative and renewable feedstocks to liquid fuels. A critical analysis of viable catalytically-based technologies will be presented. The most sustainable options will be assessed.

Mar 24, 2014 10:40 AM EB1 - Room 1011	**Dr. Ryan Chiechi** University of Groningen, the Netherlands

Contacting Molecules Using Bottom-up Nanostructures

The quasi two-dimensional nature of self-assembled monolayers (SAMs) intrinsically connects our macro world to the nano world. Research in molecular electronics is, at its core, focused on exactly this problem: how do we make contacts to molecules that are addressable from our macro world? There are numerous examples of transient contacts formed by creation various types of "break junctions" or the tip of a AFM cantilever, but making stable devices that comprise molecular tunneling junctions remains a daunting challenge.

In this talk I will discuss our efforts to combe nanoskiving (a form of edge lithography that is entirely mechanical) with SAMs to form bottom-up devices in which the smallest dimension is defined by the molecules themselves. This template approach transfers the quasi two-dimensional nature of SAMs into nano electrode architectures, enabling us to produce millimeter-long devices that are directly electrically addressable; no further lithography is required to connect these tunneling junctions to an external circuit. Typically, we use alkanedithiols as templates for forming the nano-gap devices, but we have also incorporated chromophores with large transition dipoles.

Devices formed from SAMs of these molecules exhibit photo-gating, in which the magnitude of tunneling current changes upon exposure to light. Symmetrical dithiols that are too fragile to serve as templates can be incorporated into devices via dynamic exchange, which leverages the properties of self-assembly to replace the alkanedithiol template molecules spontaneously with molecules from solution.

Mar 31, 2014 10:40 AM EB1 - Room 1011	**Dr. Charles Gersbach** Duke University

Custom Redesign of the Human Genome with Engineered DNA-Binding Proteins

The impact of reverse genetics, synthetic biology, and gene therapy has been restricted by the limitations of conventional genetic engineering technologies. To expand the capacity for genetic modification of mammalian cells, we are engineering artificial DNA-binding proteins, including zinc finger proteins, TAL effectors, and CRISPR/Cas9 to regulate and edit endogenous mammalian genes. For example, we have engineered both protein-based and RNA-guided transcriptional activators targeted to human genes relevant to medicine, science, and biotechnology.

Delivery of combinations of transcription factors led to synergistic effects on gene activation and tunable expression levels. This approach recapitulates the previously intractable complexity of natural regulation of mammalian genes that is the product of cooperative actions of many transcription factors. We have also developed novel methods for controlling the activity of these proteins, such as optogenetic regulation of protein dimerization with blue light. In other studies we have engineered synthetic nucleases to stimulate gene targeting to genomic safe harbor sites. This approach is particularly useful for generating isogenic cell lines.

We showed that this method leads to a decrease in the variability of transgene expression within a clonal cell line and between multiple clones relative to conventional techniques. Finally, we have used similar methods to correct mutations causing genetic disease. We engineered synthetic nucleases targeted to the human dystrophin gene that is mutated in Duchenne muscular dystrophy patients. When we delivered these nucleases to cells from patients with this disease, the correct gene reading frame and expression of the functional dystrophin protein were restored *in vitro* and following cell transplantation *in vivo*.

We further demonstrated that these nucleases were well-tolerated and did not lead to off-target alterations of the exome in several corrected clonal cell populations. Collectively, these studies demonstrate the potential of engineered DNA-binding proteins to enable new approaches in medicine, science, and technology.

Apr 7, 2014 10:40 AM EB1 - Room 1011	**Dr. Daeyeon Lee** University of Pennsylvania

Mechanical Properties of Nanoparticle Assemblies

Assembly of nanoparticles leads to the generation of multifunctional suprastructures with synergistic properties and performance that will drive the commercialization of nanoparticle-based products in energy conversion & storage, optics, photonics, display, water purification, sensing and biomedical applications.

One of the key bottlenecks that impede the widespread utilization of nanoparticle assemblies is their poor mechanical reliability and durability. They tend to fracture and fail under small loads. In this talk, I will describe two types of nanoparticle assemblies our group is investigating: bubbles and films. In particular, I will discuss our strategies to tailor the mechanical properties of these nanoparticle assemblies and our efforts to understand their failure modes under mechanical loads.

In the first part of this talk, I will present a new method for fabricating monodisperse nanoparticle-shelled bubbles with high mechanical properties. We demonstrate that nanoparticle shelled-bubbles, produced using microfluidics, can be reinforced using heat treatment. We characterize the mechanical properties and fracture mechanisms of nanoparticle-shelled bubbles at the single bubble level using *in situ* compression as well as *ex situ* nanoindentation. I will discuss the importance of thermal treatment on the deformation and failure modes of these nanoparticle-shelled bubbles. We also show some examples of lightweight hybrid materials that incorporate these nanoparticle shelled-bubbles.

In the second part of the talk, I will present our efforts to understand the effect of particle shape anisotropy on the mechanical behavior of disordered nanoparticle packings. We study the mechanical response of disordered nanoparticle packings made of TiO_2 prolate ellipsoids with various aspect ratios using nanoindentation. We observe striking similarities in the deformation mechanism of disordered particle assemblies to that of metallic glasses, which are random packings of metallic atoms. It is demonstrated that anisotropic particles greatly suppress shear band formation and toughen particle packings without sacrificing their strength. Our results imply that tuning constituent-anisotropy may be a new strategy to enhance toughness in disordered solids.

Apr 14, 2014 10:40 AM EB1 - Room 1011	**Dr. Gila Stein** University of Houston

Nanopatterning with Polymer Thin Films

Polymer thin films are essential for patterning microelectronics circuitry with lithographic processes. Our work explores the physical and chemical processes that drive pattern formation in two material classes that are relevant to next-generation lithography.
First, I will discuss reaction kinetics in chemically-amplified photoresists (CARs), where pattern formation is based on the acid-catalyzed deprotection of glassy polymer resins. Through a concerted experimental and modeling effort, we determined that reaction front propagation is controlled by an anomalous (subdiffusive) catalyst transport mechanism. Such behavior is associated with dynamic heterogeneities in the glassy film, which should be considered when developing high-resolution materials and predictive lithography models.
Second, I will describe nanopattern formation through block copolymer (BCP) self-assembly, a potentially inexpensive alternative to traditional lithographic approaches. Using detailed synchrotron scattering experiments, we find that interactions between the BCP and underlying substrate control defect densities, domain shapes, and domain orientations. These data demonstrate that high precision patterning by BCP self-assembly requires new strategies to formulate and define polymer-substrate interfaces.

Apr 21, 2014 10:40 AM EB1 - Room 1011	**Dr. Ah-Hyung Alissa Park** Columbia University

Towards Sustainable Energy: Carbon Capture, Utilization and Storage (CCUS)

Historically, the atmospheric concentration of CO_2 fluctuated naturally on the timescales of ice ages. Concerns, however, stem from the recent dramatic increase in CO_2 concentration, which coincides with global industrial development. This rise is mainly due to the high use of fossil fuels. In order to meet the ever-increasing global energy demands while stabilizing the CO_2 level in the atmosphere, it is widely believed that current carbon emissions must be reduced by at least a factor of three.

The containment of CO_2 involves three steps: separation, transportation, and storage. Until now, these technologies have been developed independently of one another, which has resulted in complex and economically challenging large-scale designs. The future direction of carbon management technologies now focuses on the integration of CO_2 capture and storage schemes as well as CO_2 conversion/utilization. In this seminar, two novel carbon capture, utilization and storage (CCUS) technologies will be introduced.

Nanoparticle Organic Hybrid Materials (NOHMs) are a new class of organic-inorganic hybrids that consist of a hard nanoparticle core functionalized with a molecular organic (e.g., polymeric) corona that possesses a high degree of tunability. NOHMs are non-volatile and stable over a very wide temperature range, which make them interesting materials for various energy and environmental applications.

The second set of CO_2 capture materials is derived from Mg- and Ca-bearing minerals and industrial wastes. The main advantage of carbon mineralization is that it is the most permanent and safe method of carbon storage, since the gaseous CO_2 is fixed into a solid matrix of Mg-bearing minerals (e.g., serpentine) forming a thermodynamically stable solid product. These carbon sequestration technologies can be integrated into the existing or new energy conversion systems in order to improve their overall sustainability.